

## THE CONNECTIVE ECCENTRIC INDEX FOR AN INFINITE FAMILY OF DENDRIMERS

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### ABSTRACT

Let  $G=(V,E)$  be a simple connected graph, where  $V(G)$  and  $E(G)$  be the vertex and edge sets of  $G$ . A topological index is a numeric quantity related to  $G$  which is invariant under graph automorphisms. The *Connective Eccentric index*  $C^{\xi}(G)$  is defined as  $\sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)}$  where  $d_v$  and  $\varepsilon(v)$  denote the degree of vertex  $v$  in  $G$  and the largest distance between  $v$  and any other vertex  $u$  of  $G$ . In this paper we compute the connective eccentric index for an infinite family of Nanostar Dendrimer.

**Keywords:** Nanostar Dendrimer, Connective Eccentric Index, Eccentric Connectivity Index

### INTRODUCTION

Let  $G=(V,E)$  be a simple connected molecular graph, the vertex and edge sets of a graph  $G$  are denoted by  $V(G)$  and  $E(G)$ , respectively.

Throughout this paper, graph means simple connected graph (Wiener, 1947; Gutman *et al.*, 1972; Consonni, 2000).

If  $x, y \in V(G)$  then the distance  $d(x,y)$  between  $x$  and  $y$  is defined as the length of a minimum path connecting  $x$  and  $y$ .

The *eccentric connectivity index* of the molecular graph  $G$ , was proposed by Sharma, Goswami and Madan (Sharma *et al.*, 1997). It is defined as

$$\xi(G) = \sum_{v \in V(G)} d_v \times \varepsilon(v)$$

where  $d_v$  denotes the degree of the vertex  $v$  in  $G$  and,  $\varepsilon(v)$  denote the largest distance between  $v$  and any other vertex  $u$  of  $G$  or  $\varepsilon(v) = \max\{d(v,u) \mid \forall v \in V(G)\}$ . See (Gutman *et al.*, 1986; Johnson *et al.*, 1990; Ashrafi *et al.*, 2009; Alikhani *et al.*, 2011; Ghorbani *et al.*, 2010; Kumar *et al.*, 2004; Fischermann *et al.*, 2002; Sardana *et al.*, 2001; Ashrafi *et al.*, 2009; Dureja *et al.*, 2007; YarAhmadi, 2010; Farahani 2013) for more details.

In 2000, the *Connective Eccentric index*  $C^{\xi}(G)$  of the molecular graph  $G$  was proposed by Gupta *et al.*, (2000, 2002) and is defined as:

$$C^{\xi}(G) = \sum_{v \in V(G)} \frac{d_v}{\varepsilon(v)}$$

The aim of this paper is to compute the Connective Eccentric index for an infinite family of Nanostar Dendrimer.

The Nanostar Dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. Recently some people investigated the mathematical properties of these nanostructures in (Newkome *et al.*, 2002; Heydari *et al.*, 2007; Eliasi *et al.*, 2008; Ashrafi *et al.*, 2008; Ashrafi *et al.*, 2009; Ashrafi *et al.*, 2009; Karbasioun *et al.*, 2009; Mirzagar, 2009; Alikhani *et al.*, 2010; Alikhani *et al.*, 2010; Alikhani *et al.*, 2011; Golriz *et al.*, 2011; Husin *et al.*, 2013; Farahani, 2013; Farahani, 2013; Farahani, 2015).

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### MATERIALS AND METHODS

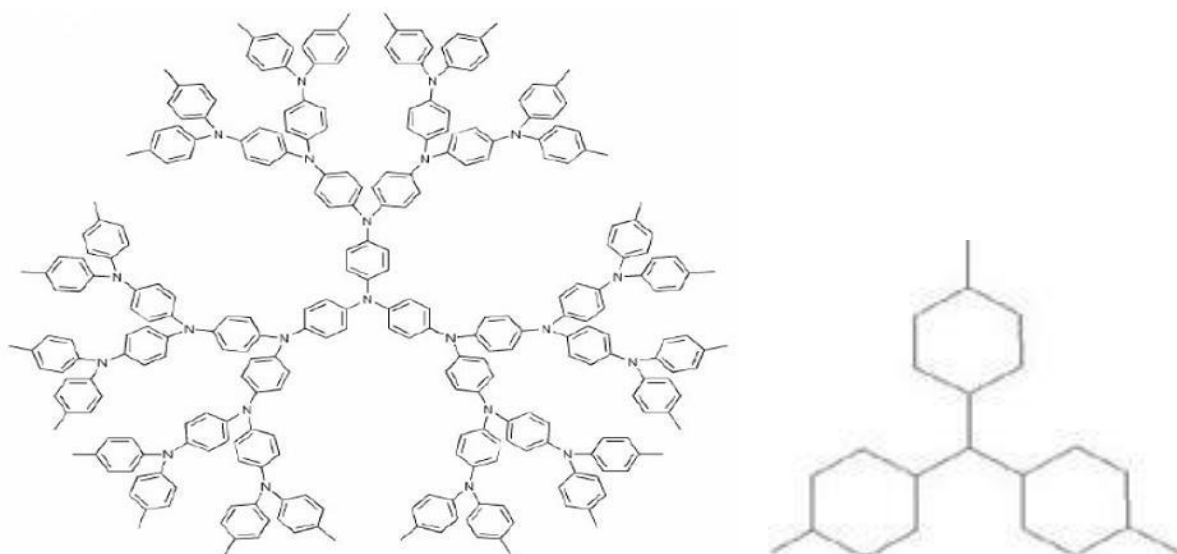
In this section, we study the Connective eccentric index  $C^c(G)$  and compute its index of an infinite family of Dendrimer.

**Theorem 1.** Let  $D_3[n]$  be the  $n^{\text{th}}$  growth of Nanostar Dendrimer ( $\forall n \geq 1$ ). Then the Connective Eccentric index  $C^c(G)$  of  $D_3[n]$  is equal to

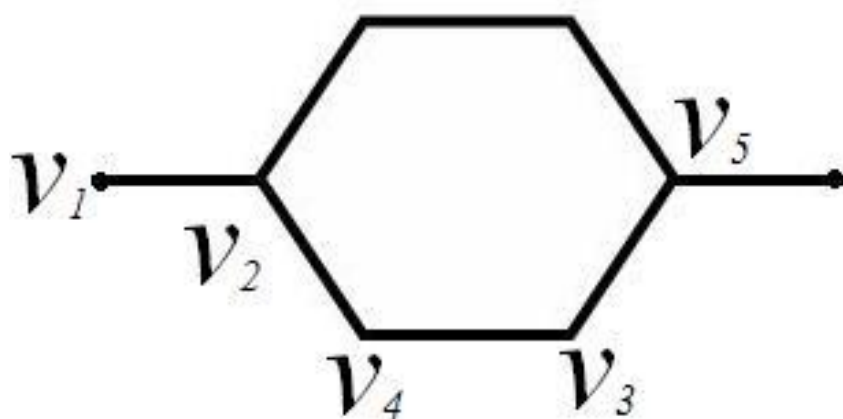
$$C^c(D_3[n]) = 3 \times \left( \sum_{i=1, \dots, n} (2^{i-1}) \left( \frac{3}{5i+5n+5} + \frac{6}{5i+5n+6} + \frac{12}{5i+5n+7} + \frac{12}{5i+5n+8} + \frac{6}{5i+5n+9} \right) + \frac{2^{n-1} - \left( \frac{2n+1}{n+2} \right)}{5(n+1)} \right)$$

**Proof of Theorem 1.**  $\forall n \in \mathbb{N} \cup \{0\}$ , consider the  $n^{\text{th}}$  growth of Nanostar Dendrimer  $D_3[n]$ .  $D_3[n]$  has  $21(2^{n+1}) - 20$  vertices/atoms and  $24(2^{n+1} - 1)$  bonds/edges (see Figure 1). For further study and more detail of this Benzenoid family, see the paper series (Husin *et al.*, 2013; Farahani, 2013; Farahani, 2013; Farahani, 2015).

The Nanostar Dendrimer  $D_3[n]$  has a core depicted in Figure 1 and we define an element as Figure 2 by "Leaf".



**Figure 1:** The first kind of Dendrimer of generation 1-3 has grown 3 stages and  $D_3[0]$  is the primal structure of Nanostar Dendrimer  $D_3[n]$ .



**Figure 2:** The added graph in each branch of  $D_3[n]$ .

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It is obvious that a leaf consist of a cycle  $C_6$  and add  $3(2^n)$  leafs to  $D_3[n-1]$  in the  $n^{th}$  growth of Nanostar Dendrimer. Therefore, there exist the number of  $\xi_n = 3 \sum_{i=0}^n (2^i) = 3 \left( \frac{2^{n+1}-1}{2-1} \right)$  of leafs ( $C_6$ ) in Nanostar

Dendrimer  $D_3[n]$ .

Consider the  $n-1^{th}$  growth of Nanostar Dendrimer in  $D_3[n-1]$  and we would like to construct  $D_3[n]$ . In every branch of  $D_3[n]$ , the leaf graph added. From Figure 2, one can see that the maximum eccentricity of a leaf of  $D_3[n]$  is 6, and also, the eccentricity of previous vertices of core  $D_3[0]$  are equal to 10.

Thus, for eccentric of vertices in added leaf of Nanostar Dendrimer  $D_3[n-1]$  to  $D_3[n]$ , we can following results:

We have  $3(2^{n-1})$  vertices of kind labeled  $v_1$  with eccentricity  $5n+5(n+1)$  and have  $3(2^n)$  vertices of kind labeled  $v_2$  with eccentricity  $5n+1+5(n+1)$ .

Also there are  $3(2^{n+1})$  vertices of  $v_3$  and  $v_4$ , with eccentricity  $10n+7$  and  $5n+8$ , respectively. And  $3(2^n)$  vertices  $v_5$ , its eccentricity is  $10n+9$ .

Also, from the general representation of Nanostar Dendrimer  $D_3[n]$  in Figure 1, it is easy to see that all Hydrogen atoms in added leafs have degree 1 and all other vertices/atoms have degree three.

Thus, we have following computations for the Connective Eccentric index  $C^e$  of the  $n^{th}$  growth of Nanostar Dendrimer  $D_3[n]$ ,  $\forall n \in \mathbb{N}$  as:

$$\begin{aligned} C^e(D_3[n]) &= \sum_{v \in V(D_3[n])} \frac{d_v}{\varepsilon(v)} \\ &= \sum_{\substack{\text{vertex labeled } v_1 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{d_{v_1}}{\varepsilon(v_1)} + \sum_{\substack{\text{vertex labeled } v_2 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{d_{v_2}}{\varepsilon(v_2)} + \sum_{\substack{\text{vertex labeled } v_3 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{d_{v_3}}{\varepsilon(v_3)} \\ &+ \sum_{\substack{\text{vertex labeled } v_4 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{d_{v_4}}{\varepsilon(v_4)} + \sum_{\substack{\text{vertex labeled } v_5 \text{ in } D_3[i] \\ i=1, \dots, n}} \frac{d_{v_5}}{\varepsilon(v_5)} + \sum_{\substack{\text{Hydrogen atoms of } D_3[n]}} \frac{d_H}{\varepsilon(H)} \\ &= \frac{3}{5n+5} + \sum_{i=2, \dots, n} 3(2^{i-1}) \frac{3}{5i+5n+5} + \sum_{i=1, \dots, n} 3(2^i) \frac{3}{5i+5n+6} + \sum_{i=1, \dots, n} 3(2^{i+1}) \frac{2}{5i+5n+7} \\ &+ \sum_{i=1, \dots, n} 3(2^{i+1}) \frac{2}{5i+5n+8} + \sum_{i=1, \dots, n} 3(2^i) \frac{3}{5i+5n+9} + \frac{3(2^n)}{10(n+1)} \\ &= \sum_{i=1, \dots, n} \frac{3^2(2^{i-1})}{5i+5n+5} + \sum_{i=1, \dots, n} \frac{3^2(2^i)}{5i+5n+6} + \sum_{i=1, \dots, n} \frac{3(2^{i+2})}{5i+5n+7} + \sum_{i=1, \dots, n} \frac{3(2^{i+2})}{5i+5n+8} \\ &+ \sum_{i=1, \dots, n} \frac{3^2(2^i)}{5i+5n+9} + \frac{3(2^n)}{10(n+1)} - \frac{3(2n+1)}{5(n^2+3n+2)} \\ &= 3 \times \left( \sum_{i=1, \dots, n} (2^{i-1}) \left( \frac{3}{5i+5n+5} + \frac{6}{5i+5n+6} + \frac{12}{5i+5n+7} + \frac{12}{5i+5n+8} + \frac{6}{5i+5n+9} \right) + \frac{2^{n-1} - (2n+1/n+2)}{5(n+1)} \right) \end{aligned}$$

And this completed the proof of Theorem 1.  $\square$

Reader can see some values of the Connective Eccentric index  $C^e$  of  $D_3[n]$  for integer  $n=1, 2, 3, \dots, 1000$  in following table.

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**Table 1: Some values of the Connective Eccentric index  $C^{\xi}(D_3[n])$  for integer  $n=1, 2, 3, \dots, 1000$**

$n$	$ V(D_3[n]) $	$ E(D_3[n]) $	Connective Eccentric index $C^{\xi}(D_3[n])$
1	64	72	6.79001547987616
2	148	168	13.9928138178663
3	316	360	24.490067851166
4	652	744	41.550751144813
5	1324	1512	117.660936869584
6	2668	3048	121.30647812691
7	5356	6120	211.314999770378
8	10732	12264	373.056233480523
9	21484	24552	666.56944159841
10	42988	49128	1203.57519017428
20	44040172	50331624	622223.87780502
30	45097156588	51539607528	426199600.797565
40	46179488366572	52776558133224	327912915489.941
50	4.72877960873902E16	5.40431955284459E16	268928103252621
60	4.84227031934876E19	5.53402322211287E19	2.2966089766362E17
70	4.95848480701313E22	5.66683977944357E22	2.01688378022574E20
80	5.07748844238144E25	5.80284393415022E25	1.8078866983509E23
90	5.1993481649986E28	5.94211218856983E28	1.64612017251685E26
100	5.32413252095856E31	6.0847228810955E31	1.51746610005702E29
200	6.74913978588776E61	7.71330261244315E61	9.61943682075734E58
300	8.55555110060484E91	9.77777268640553E91	8.13551180348495E88
400	1.0845449487965E122	1.23947994148172E122	7.73769523182308E118
500	1.37482405531638E152	1.57122749179015E152	7.84876851937877E148
600	1.74279653893002E182	1.99176747306288E182	8.29253049846576E178
700	2.20925707865032E212	2.52486523274322E212	9.01131242489797E208
800	2.80056606180954E242	3.20064692778233E242	9.99613017109719E238
900	3.55013924923167E272	4.05730199912191E272	1.12643772146726E269
1000	4.50033615018232E302	5.14324131449408E302	1.28520346166618E299

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## REFERENCES

- Alikhani S and Iranmanesh MA (2010).** Chromatic polynomials of some Dendrimers. *Journal of Computational and Theoretical Nanoscience* **7**(11) 2314-2316.
- Alikhani S and Iranmanesh MA (2010).** Chromatic polynomials of some Nanostars. *Iranian Journal of Mathematical Chemistry* **3**(2) 127-135.
- Alikhani S and Iranmanesh MA (2011).** Eccentric connectivity polynomials of an infinite family of Dendrimer. *Digest Journal of Nanomaterials and Biostructures* **6**(1) 256-257.
- Ashrafi AR and Mirzargar M (2008).** PI, Szeged, and edge Szeged indices of an infinite family of Nanostar Dendrimers. *Indian Journal of Chemistry* **47** 538-541.
- Ashrafi AR and Nikzad P (2009).** Connectivity index of the family of Dendrimer Nanostars. *Digest Journal of Nanomaterials and Biostructures* **4**(2) 269-273.

## Research Article

- Ashrafi AR and Nikzad P (2009).** Kekule index and bounds of energy for Nanostar Dendrimers. *Digest Journal of Nanomaterials and Biostructures* **4**(2) 383-388
- Ashrafi AR, Ghorbani M and Hemmasi M (2009).** Eccentricity Connectivity Polynomial of  $C_{12n+2}$  Fullerenes. *Digest Journal of Nanomaterials and Biostructures* **4**(3) 483-486.
- Ashrafi AR, Ghorbani M and Jalali M (2009).** Eccentric connectivity polynomial of an infinite family of Fullerenes. *Optoelectronics and Advanced Materials: Rapid Communications* **3** 823-826.
- Dureja H and Madan AK (2007).** Super augmented eccentric connectivity indices: highly discriminating topological descriptors for QSAR/QSPR modeling. *Medicinal Chemistry Research* **16** 331–341.
- Eliasi M and Taeri B (2008).** Szeged index of armchair polyhex nanotubes. *MATCH: Communications in Mathematical and in Computer Chemistry* **59**(2) 437-450.
- Farahani MR (2013).** Computing Eccentricity Connectivity Polynomial of Circumcoronene Series of Benzenoid  $H_k$  by Ring-Cut Method. *Annals of West University of Timisoara-Mathematics and Computer Science* **51**(2) 29–37.
- Farahani MR (2013).** Computing Fifth Geometric-Arithmetic Index of Dendrimer Nanostars. *Advances in Materials and Corrosion* **1** 62-64.
- Farahani MR (2013).** Fourth atom-bond connectivity index of an infinite class of Nanostar Dendrimer  $D_3[n]$ . *Journal of Advances in Chemistry* **4**(1) 301-305.
- Farahani MR (2015).** Some Connectivity index of an infinite class of Dendrimer Nanostars. *Journal of Applied Physical Science International* **3**(3) 99-105.
- Fischermann M, Homann A, Rautenbach D, Szekely LA and Volkmann L (2002).** Wiener index versus maximum degree in trees. *Discrete Applied Mathematics* **122** 127–137.
- Ghorbani M and Ghazi M (2010).** Computing Some Topological Indices of Triangular Benzenoid. *Digest Journal of Nanomaterials and Biostructures* **5**(4) 1107-1111.
- Golriz M, Darafsheh MR and Khalifeh MH (2011).** The Wiener, Szeged and PI-indices of a phenylazomethine Dendrimer. *Digest Journal of Nanomaterials and Biostructures* **6**(4) 1545-1549.
- Gupta S, Singh M and Madan AK (2000).** Connective eccentricity Index: A novel topological descriptor for predicting biological activity. *Journal of Molecular Graphics and Modelling* **18** 18–25.
- Gupta S, Singh M and Madan AK (2002).** Application of graph theory: Relationship of eccentric connectivity index and Wiener's index with anti-inflammatory activity. *Journal of Mathematical Analysis and Applications* **266** 259-268.
- Gutman I and Polansky OE (1986).** *Mathematical Concepts in Organic Chemistry* (Springer-Verlag, New York).
- Gutman I and Trinajstić N (1972).** Graph theory and molecular orbitals. *Chemical Physics Letters* **17** 535–538.
- Heydari A and Taeri B (2007).** Szeged index of  $TUC_4C_8$  (R) nanotubes. *MATCH: Communications in Mathematical and in Computer Chemistry* **57**(2) 463-477.
- Husin NM, Hasni R and Arif NE (2013).** Atom-Bond Connectivity and Geometric Arithmetic Indices of Dendrimer Nanostars. *Australian Journal of Basic and Applied Sciences* **7**(9) 10-14.
- Johnson MA and Maggiora GM (1990).** *Concepts and Applications of Molecular Similarity* (Wiley Interscience, New York).
- Karbasioun A and Ashrafi AR (2009).** Wiener and detour indices of a new type of Nanostar Dendrimers. *Macedonian Journal of Chemistry and Chemical Engineering* **28**(1) 49-54
- Kumar V, Sardana S and Madan AK (2004).** Predicting anti- HIV activity of 2,3-diary 1-1,3-thiazolidin-4-ones: computational approaches using reformed eccentric connectivity index. *Journal of Molecular Modeling* **10** 399–407.
- Mirzagar M (2009).** PI, Szeged and edge Szeged polynomials of a Dendrimer Nanostar. *MATCH: Communications in Mathematical and in Computer Chemistry* **62** 363-370.
- Newkome GR, Moorefield CN and Vogtlen F (2002).** *Dendrimer and Dendrons: Concepts, Syntheses, Applications* (Wiley-VCH Verlag GmbH & Co. KGaA).

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**Sardana S and Madan AK (2001).** Application of graph theory: Relationship of molecular connectivity index, Wiener's index and eccentric connectivity index with diuretic activity. *MATCH: Communications in Mathematical and in Computer Chemistry* **43** 85-89.

**Sharma V, Goswami R and Madan AK (1997).** Eccentric connectivity index: a novel highly of descriptor for structure-property and structure-activity studies. *Journal of Chemical Information and Computer Sciences* **37** 273– 282.

**Todeschini R and Consonni V (2000).** *Handbook of Molecular Descriptors* (Wiley, Weinheim).

**Wiener H (1947).** Structural determination of the paraffin boiling points. *Journal of the American Chemical Society* **69** 17–20.

**YarAhmadi Z (2010).** Eccentric connectivity and augmented of N-branches phenylacetylenes Nanostar Dendrimers. *Iranian Journal of Mathematical Chemistry* **1**(2) 105– 110.